Supporting Information

A particle-scale reduction analysis of $CuFeMnO_4$ with hydrogen for chemical looping combustion

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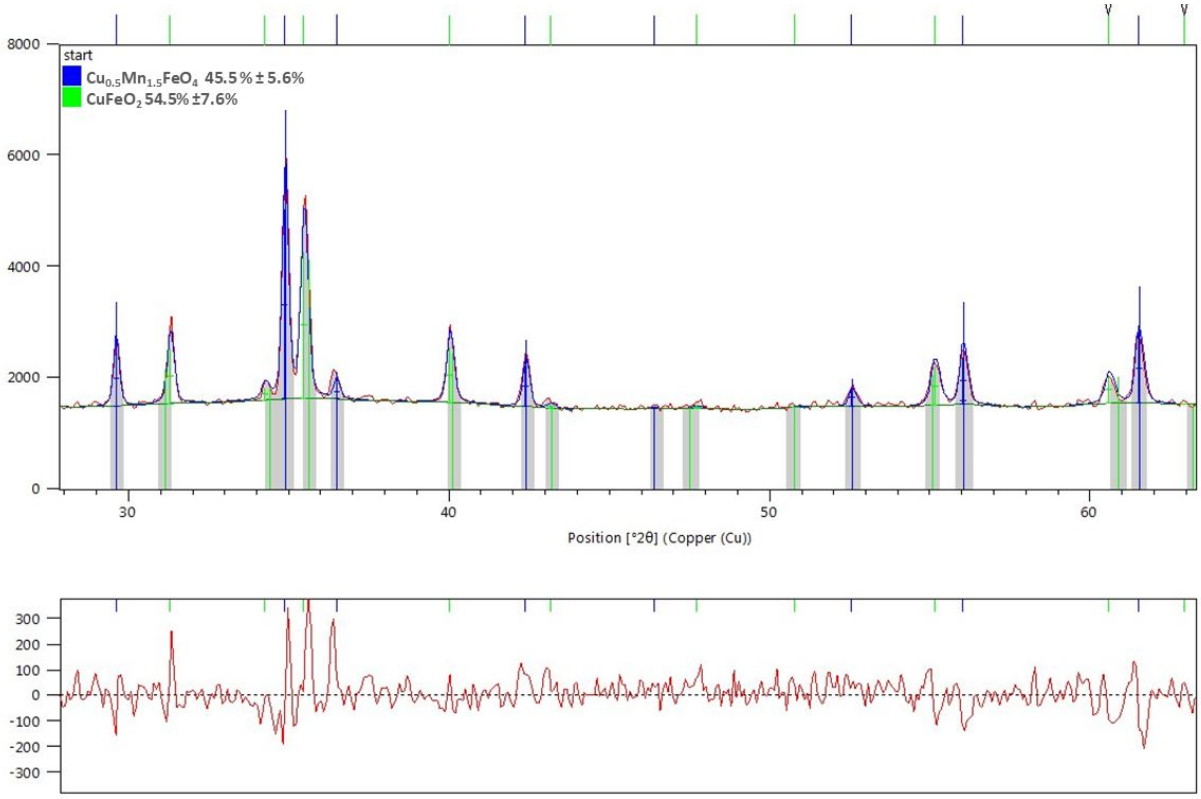

(c)	$CuFeO_2$	$Cu_{0.5}Mn_{1.5}FeO_4$
Unit Cell		
a [Å]	**3.053**	**8.518**
b [Å]	**3.053**	**8.518**
c [Å]	**17.119**	**8.518**
alpha [°]	**90**	**90**
beta [°]	**90**	**90**
ganna [°]	**120**	**90**
Atom Positions		
Cu1 (x,y,z), Occupancy	**(0,0,0), 1**	**(0,0,0), 0.245**
Cu2 (x,y,z), Occupancy	**N/A**	**(0.375, 0.375, 0.375), 0.01**
Fe1 (x,y,z), Occupancy	**(0,0,0.5), 1**	**(0,0,0), 0.25**
Fe2 (x,y,z), Occupancy	**N/A**	**(0.375, 0.375, 0.375), 0.5**
Mn1 (x,y,z), Occupancy	**N/A**	**(0.375, 0.375, 0.375), 0.49**
Mn2 (x,y,z), Occupancy	**N/A**	**(0, 0, 0), 0.505**
O1 (x,y,z), Occupancy	**(0,0,0.101), 1**	**(0.2412, 0.2412, 0.2412), 1**

Figure S1: Analysis of $CuFeO_2$ and $Cu_{0.5}Mn_{1.5}FeO_4$ phase fit for Composition of phases during reaction modeling (a), residual error analysis (b), and reported lattice parameters and atom positions for the dual phase system (c).

Table S1. Theoretical enthalpies (FactSage) of reactions with H_2 and metal oxides

Reaction	ΔH_{800} (kJ)/mole H_2
$2\ CuO + H_2 \rightarrow Cu_2O + H_2O$	-116.0
$Cu_2O + H_2 \rightarrow 2\ Cu + H_2O$	-81.1
$3\ Fe_2O_3 + H_2 \rightarrow 2\ Fe_3O_4 + H_2O$	-5.3
$Fe_3O_4 + H_2 \rightarrow 3\ FeO + H_2O$	+50.5
$FeO + H_2 \rightarrow Fe + H_2O$	+16.1 *$\Delta G_{800} > 0$
$3\ Mn_2O_3 + H_2 \rightarrow 2\ Mn_3O_4 + H_2O$	-176.1
$Mn_3O_4 + H_2 \rightarrow 3\ MnO + H_2O$	-19.7
$MnO + H_2 \rightarrow Mn + H_2O$	+137.6 *$\Delta G_{800} > 0$

Table S2. Theoretical and experimental oxygen transfer capacities (OTC) of $CuFeMnO_4$ and constituent metal oxides

Reaction	OTC_{th}	OTC_{expt}
$CuO + Fe_3O_4 + Mn_3O_4 + 6\ H_2 \rightarrow Cu + 3\ MnO + 3\ Fe + 6\ H_2O$	17.9 %	18.3 %
$CuFeMnO_4 + 2{,}3\ H_2 \rightarrow CuFeMnO_2/CuFeMnO + 2{,}3\ H_2O$	13.4 % - 20.1 %	18.3 %
$CuO + H_2 \rightarrow Cu + H_2O$	20.1 %	20.1 %
$Fe_2O_3 + 3\ H_2 \rightarrow 2\ Fe + 3\ H_2O$	30.1 %	28.0 %
$Mn_2O_3 + H_2 \rightarrow 2\ MnO + H_2O$	10.1 %	8.6 %

*th = theoretical , expt = experimental

Table S3. Theoretical and experimental OTC of $CuFeMnO_4$ and bi-metallics

Reaction	OTC_{th}	OTC_{expt}
$CuO + Fe_3O_4 + Mn_3O_4 + 3\ H_2 \rightarrow Cu + 3\ Fe + 3\ MnO + 3H_2O$	17.9%	18.3%
$CuFeMnO_4 + 3(4/3)\ H_2 \rightarrow Cu + Fe/(1/3)Fe_3O_4 + MnO + 3(4/3)\ H_2O$	11.1%-20.1%	18.3%
$CuFe_2O_4 + 4(2)H_2 \rightarrow Cu + 2Fe/FeO + 4(2)H_2O$	15.1%-25.1%	23.6%
$CuMn_2O_4 + 2H_2 \rightarrow Cu + 2MnO + 2H_2O$	15.1%	15.4%
$Fe_2O_3 + Mn_2O_3 + 3(2)H_2 \rightarrow 2Fe/FeO + 2MnO + 3(2)H_2O$	10.1%-20.0%	17.0%